

## **General Disclaimer**

### **One or more of the Following Statements may affect this Document**

- This document has been reproduced from the best copy furnished by the organizational source. It is being released in the interest of making available as much information as possible.
- This document may contain data, which exceeds the sheet parameters. It was furnished in this condition by the organizational source and is the best copy available.
- This document may contain tone-on-tone or color graphs, charts and/or pictures, which have been reproduced in black and white.
- This document is paginated as submitted by the original source.
- Portions of this document are not fully legible due to the historical nature of some of the material. However, it is the best reproduction available from the original submission.

NASA Contractor Report 168337

An Interactive Computer Code for Calculation of Gas-Phase Chemical  
Equilibrium (EQLBRM)

Brian S. Pratt and David T. Pratt

University of Washington  
Seattle, Washington

(NASA-CR-168337) AN INTERACTIVE COMPUTER  
CODE FOR CALCULATION OF GAS-PHASE CHEMICAL  
EQUILIBRIUM (EQLBRM) Final Report  
(Washington Univ.) 22 p HC A02/MF A01

N85-10948

Unclas  
CSCL 21E G3/07 24379

October 1984



Prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION  
Lewis Research Center  
Under Grant NAG 3-277

## PREFACE

This report describes EQLBRM, an interactive FORTRAN-IV computer program for computing adiabatic flame temperatures and equilibrium product composition for the combustion of hydrocarbon fuels in air. The authors are grateful to Paul S. Cramer of the AVCO-Lycoming Corporation for extensively testing EQLBRM and suggesting many improvements.

## TABLE OF CONTENTS

PREFACE . . . . .	1
1. INTRODUCTION . . . . .	1
1.1 Overview . . . . .	1
1.2 Method of Solution . . . . .	1
1.3 Special Features . . . . .	1
1.4 Limitations . . . . .	1
2. USER'S GUIDE . . . . .	2
2.1 Example Run 1 . . . . .	2
2.2 Example Run 2 . . . . .	5
2.3 Debugging . . . . .	14
2.4 FORTRAN Language and Availability . . . . .	14
3. THERMOCHEMICAL DATA . . . . .	15
4. REFERENCES . . . . .	19

PRECEDING PAGE BLANK NOT FILMED

## 1. INTRODUCTION

### 1.1 Overview

EQLBRM is a user-friendly, menu-driven, interactive computer program which calculates the adiabatic equilibrium temperature and product composition resulting from the combustion of hydrocarbon fuels with air, at specified constant pressure and enthalpy. EQLBRM was developed primarily as an instructional tool to be run on small computers to allow the user to economically and efficiently explore the effects of varying fuel type, air-fuel ratio, inlet air and/or fuel temperature, and operating pressure on the performance of continuous combustion devices such as gas turbine combustors, Stirling engine burners, and power-generation furnaces.

### 1.2 Method of Solution

EQLBRM is based on the principle of minimization of the Gibbs function of a reactive mixture at constant pressure, subject to constraints of conservation of atomic species and enthalpy. The minimization algorithm used is the very efficient and robust Gordon and McBride method (ref. 1), as refined and simplified by Pratt (refs. 2 to 4), and recently developed independently by Reynolds (ref. 5). A detailed description of the solution algorithm is contained in reference 4.

### 1.3 Special Features

The many "user-friendly" features offered by EQLBRM include:

1. A resident default combustion problem specification allows immediate demonstration of program execution and output format.
2. Interactive, run-time selection of SI or English units.
3. Fuel compounds may be either chosen from a resident data file, EQLBRM.DAT, or entered interactively at run time.
4. Composition of the adiabatic equilibrium combustion products is output in mole numbers, mole fractions, mass fractions and emission index.
5. At the user's option, a summary of the inlet conditions together with the equilibrium solution may be written to a file, EQLOUT.LST, for subsequent hard copy output.

### 1.4 Limitations

Compared to the powerful NASA equilibrium code CEC71(1), EQLBRM has the following limitations:

1. To fit in a small computer, program size is limited to 80 species, compared to over 500 species in CEC71. (The limitation to 80 species includes any new species added during an interactive session.)
2. Condensed species are not considered.

3. Only the HP problem (assigned enthalpy and pressure) is considered by EQLBRM, while CEC71 considers also the TP, UV, TV, SP and SV problems (ref. 1).

4. Multiple problem statements are not considered.

5. EQLBRM considers only the first NPROD species in the THERMO data file (see Chapter 3) as combustion products; NPROD is presently hard-coded as 11. NPROD can be modified only by altering a DATA statement in the BLOCK DATA sub-program source code.

## 2. USER'S GUIDE

A well-written interactive program contains the equivalent of a User's Guide in its interactive menu structure and prompts. As a practical matter, it is necessary to actually use an interactive program to discover how it works. One way to resolve this "Catch-22" dilemma is to obtain telephone-line access to a demonstration run on a computer in which the interactive program is installed. By this method a prospective user can "take a test drive" and see whether or not the program is of further interest.

An alternative method is the presentation of example interactive sessions. Two such example sessions are presented here. In both examples, everything that would appear on the user's terminal (either a printing terminal or cathode-ray tube screen) appears in UPPER CASE text, as it does in actual program execution. The user response to prompts is boxed, and the lower case text are comments provided to rationalize the hypothetical user's choices, or to highlight some of the features of EQLBRM.

### 2.1 Example Run 1

In this example, it is assumed that the user is running EQLBRM for the first time, and wishes only to become familiar with its operation, rather than solve a specific problem. The user therefore types in "RUN EQLBRM" or an equivalent system command to execute the compiled and linked load module named "EQLBRM."

Immediately EQLBRM introduces itself by printing to the terminal:

\*\*\* PROGRAM EQLBRM \*\*\*

CALCULATES THE ADIABATIC EQUILIBRIUM TEMPERATURE AND PRODUCT COMPOSITION  
RESULTING FROM COMBUSTION OF HYDROCARBON FUELS AND AIR AT CONSTANT PRES-  
SURE AND ENTHALPY.

USER MUST SPECIFY INITIAL FUEL COMPOSITION AND TEMPERATURE, INITIAL AIR  
TEMPERATURE, AIR-FUEL MIXTURE RATIO, AND PRESSURE. A VARIETY OF UNITS ARE  
AVAILABLE:

TEMPERATURE	PRESSURE	AIR-FUEL RATIO
KELVIN	KILO PASCALS	KG AIR/KG FUEL
CELSIUS	P.S.I.	KG FUEL/KG AIR
FAHRENHEIT	ATMOSPHERES	MOLS AIR/MOLS FUEL
RANKINE	BAR	MOLS FUEL/MOLS AIR
		FUEL-AIR EQUIVALENCE RATIO

EQLBRM WILL RETURN THE EQUILIBRIUM TEMPERATURE AND FUEL-AIR EQUIVALENCE RATIO, AS WELL AS THE MOLE NUMBER, MOLE FRACTION, MASS FRACTION AND EMISSION INDEX OF THE PRODUCTS AT EQUILIBRIUM.

PRESS <RETURN> TO CONTINUE

Being an interactive program, EQLBRM always prompts the user for the proper response or range of responses. The user responds with:

IF THE USER SPECIFIES A FUEL FOR WHICH EQLBRM HAS NO THERMOCHEMICAL DATA, THE USER MAY EXPLICITLY SUPPLY THE FUEL CHEMICAL FORMULA AND STANDARD STATE ENTHALPY OF FORMATION OR LOWER HEATING VALUE. AGAIN, A CHOICE OF UNITS WILL BE AVAILABLE TO THE USER.

WOULD YOU LIKE TO SEE A SAMPLE DATA SET (Y/N)

Since this is just a familiarization run, the user elects to inspect the sample data set.

\*\*\*CURRENT DATA STATUS\*\*\*

FUELS AND FUEL AMOUNTS :

FUEL	RELATIVE MOLES AMONG FUELS
CO	1.0000000
H2	2.0000000

FUEL TEMP = 2.9800E+02 DEG- KELVIN

AIR TEMP = 7.5000E+02 DEG- KELVIN

PRESSURE = 5.0000E+00 ATMOSPHERES

A-F RATIO = 8.5000E-01 FUEL-AIR EQUIVALENCE RATIO

SELECT AN OPTION:

0- RUN WITH THIS DATA

1- CHANGE FUELS OR FUEL AMOUNTS

2- CHANGE FUEL TEMPERATURE

3- CHANGE AIR TEMPERATURE

4- CHANGE TEMPERATURE UNITS

5- CHANGE PRESSURE OR PRESSURE UNITS

6- CHANGE AIR-FUEL RATIO OR RATIO UNITS

OPTION NUMBER? (0-6)

Again, since this is just a familiarization run, the user chooses to run with the sample data set, just to see what the output looks like.

RUN WITH THIS DATA: ARE YOU SURE? (Y/N)

EQLBRM always double-checks before execution to avoid possible time-costly user error.

☒ Y

Now EQLBRM executes the sample data set and returns the solution to the screen:

\*\*\*\*\*  
OUTPUT  
\*\*\*\*\*

\*\*\* ADIABATIC EQUILIBRIUM AT CONSTANT PRESSURE AND ENTHALPY \*\*\*

PRESSURE= 5.000E+00 ATMOSPHERES  
TEMPERATURE = 2444.76 DEGREES KELVIN  
FUEL-AIR EQUIVALENCE RATIO = 0.850

SPECIES NAME ("I")	MOLE NUMBER (MOL-I/G-X)	MOLE FRACTION (MOL-I/MOL-X)	MASS FRACTION (G-I/G-X)	EMISSION INDEX (G-I/KG-FUEL)
CO	2.204E-04	6.078E-03	6.173E-03	6.173E+00
CO2	3.270E-03	9.019E-02	1.439E-01	1.439E+02
H	1.458E-05	4.020E-04	1.469E-05	1.469E-02
H2	7.696E-05	2.123E-03	1.551E-04	1.551E-01
H2O	6.771E-03	1.868E-01	1.220E-01	1.220E+02
N	2.282E-09	6.292E-08	3.196E-08	3.196E-05
NO	2.848E-04	7.854E-03	8.545E-03	8.545E+00
N2	2.417E-02	6.667E-01	6.772E-01	6.772E+02
O	3.161E-05	8.719E-04	5.058E-04	5.058E-01
OH	2.503E-04	6.903E-03	4.257E-03	4.257E+00
O2	1.163E-03	3.209E-02	3.723E-02	3.723E+01

DO YOU WANT A HARD COPY OF YOUR INPUT AND OUTPUT? (Y/N)

The user elects to make a hardcopy of both the input and output datasets.

☒ Y

DATA AND RESULTS ARE BEING APPENDED TO  
FILE "EQLOUT.LST" IN YOUR DIRECTORY.

The hard copy output is directed to logical unit 2. System-specific commands must be executed at run time (or added to the source code) to assign this unit to the file "EQLOUT.LST," or directly to a printer.

DO YOU WANT ANOTHER RUN? (Y/N)

A "Y" response would return the user to the main input menu, where the current input conditions can be modified interactively, as demonstrated in the next example run. However, the user in this case chooses to end the familiarization session.

☐ N



## 2.2 Example Run 2

In this example, we assume the user wishes to solve the following problem: Propane at 125° C burns with air at 375° C, at constant pressure of 4.5 atmospheres, with a slightly rich fuel-air equivalence ratio of 1.1.

The user initiates EQLBRM, and the program introduces itself:

\*\*\* PROGRAM EQLBRM \*\*\*

CALCULATES THE ADIABATIC EQUILIBRIUM TEMPERATURE AND PRODUCT COMPOSITION RESULTING FROM COMBUSTION OF HYDROCARBON FUELS AND AIR AT CONSTANT PRESSURE AND ENTHALPY.

USER MUST SPECIFY INITIAL FUEL COMPOSITION AND TEMPERATURE, INITIAL AIR TEMPERATURE, AIR-FUEL MIXTURE RATIO, AND PRESSURE. A VARIETY OF UNITS ARE AVAILABLE:

TEMPERATURE	PRESSURE	AIR-FUEL RATIO
KELVIN	KILO PASCALS	KG AIR/KG FUEL
CELSIUS	P.S.I.	KG FUEL/KG AIR
FAHRENHEIT	ATMOSPHERES	MOLS AIR/MOLS FUEL
RANKINE	BAR	MOLS FUEL/MOLS AIR
		FUEL-AIR EQUIVALENCE RATIO

EQLBRM WILL RETURN THE EQUILIBRIUM TEMPERATURE AND FUEL-AIR EQUIVALENCE RATIO, AS WELL AS THE MOLE NUMBER, MOLE FRACTION, MASS FRACTION AND EMISSION INDEX OF THE PRODUCTS AT EQUILIBRIUM.

PRESS <RETURN> TO CONTINUE.

IF THE USER SPECIFIES A FUEL FOR WHICH EQLBRM HAS NO THERMOCHEMICAL DATA, THE USER MAY EXPLICITLY SUPPLY THE FUEL CHEMICAL FORMULA AND STANDARD STATE ENTHALPY OF FORMATION OR LOWER HEATING VALUE. AGAIN, A CHOICE OF UNITS WILL BE AVAILABLE TO THE USER.

WOULD YOU LIKE TO SEE A SAMPLE DATA SET? (Y/N)

Since the user has a data set in mind already, there is no interest in seeing the sample dataset.

\*\*\*CURRENT DATA STATUS\*\*\*

FUELS AND FUEL AMOUNTS :  
FUEL                      RELATIVE MOLES AMONG FUELS  
- NO FUEL SPECIFIED -  
FUEL TEMP = 0.0000E-01 DEG- KELVIN  
AIR TEMP = 0.0000E-01 DEG- KELVIN  
PRESSURE = 0.0000E-01 ATMOSPHERES  
A-F RATIO = 0.0000E-01 FUEL-AIR EQUIVALENCE RATIO

SELECT AN OPTION:  
0- RUN WITH THIS DATA  
1- CHANGE FUELS OR FUEL AMOUNTS  
2- CHANGE FUEL TEMPERATURE  
3- CHANGE AIF TEMPERATURE  
4- CHANGE TEMPERATURE UNITS  
5- CHANGE PRESSURE OR PRESSURE UNITS  
6- CHANGE AIR-FUEL RATIO OR RATIO UNITS

OPTION NUMBER? (0-6)

Note that the main input menu comes up blank. Data must be entered by the user interactively. The order in which this is done is not important, only it is important that no null data be left when the dataset is executed. For the sake of convenience, the user decides to begin with option 1, and work down:

**1**

\*CURRENT FUELS DATA\*

FUEL                    RELATIVE MOLES AMONG FUELS  
- NO FUEL SPECIFIED -

SELECT AN OPTION:  
0- NO MORE CHANGES HERE  
1- CHANGE RELATIVE MOLES OF AN EXISTING FUEL  
2- ADD A NEW FUEL  
3- REMOVE AN EXISTING FUEL  
4- LIST ALL COMPOUNDS AVAILABLE IN THE THERMO LIBRARY

OPTION? (0-4)

The user is now in the fuels sub-menu, and exercises the 2nd option - logically enough.

**2**

ENTER NEW FUEL NAME.

The user could enter any alphanumeric string here - but EQLBRM is looking for a chemical formula. We assume the user carelessly enters "C7H8" as propane:

**C7H8**

ENTER RELATIVE MOLES OF C7H8

If there is to be a mixture of fuels, it is necessary to specify the relative amount of each fuel. For the case of a single fuel, however, any nonzero value will do. The user chooses "1.0."

**1.00**

\*CURRENT FUELS DATA\*

FUEL                    RELATIVE MOLES AMONG FUELS  
C7H8                    1.0000E+00

SELECT AN OPTION:

- 0- NO MORE CHANGES HERE
- 1- CHANGE RELATIVE MOLES OF AN EXISTING FUEL
- 2- ADD A NEW FUEL
- 3- REMOVE AN EXISTING FUEL
- 4- LIST ALL COMPOUNDS AVAILABLE IN THE THERMO LIBRARY

OPTION. (0-4)

The user notices the error that propane is C3H8, not C7H8 as entered. Option 3 must be exercised to remove the erroneous fuel selection.

DELETE C7H8

-- ARE YOU SURE? (Y/N)

EQLBRM double checks with the user in order to avoid time-consuming deletion errors.

\*CURRENT FUELS DATA\*

FUEL                    RELATIVE MOLES AMONG FUELS  
- NO FUEL SPECIFIED -

SELECT AN OPTION:

- 0- NO MORE CHANGES HERE
- 1- CHANGE RELATIVE MOLES OF AN EXISTING FUEL
- 2- ADD A NEW FUEL
- 3- REMOVE AN EXISTING FUEL
- 4- LIST ALL COMPOUNDS AVAILABLE IN THE THERMO LIBRARY

OPTION? (0-4)

Option 2 is used again to enter the correct fuel name.

ENTER NEW FUEL NAME.

-- SORRY -- C3H8  
IS NOT IN THE THERMOCHEMICAL LIBRARY. IF YOU WISH TO USE THIS COMPOUND  
YOU WILL HAVE TO SPECIFY THE ENTHALPY OF FORMATION OR LOWER HEAT VALUE.  
DO YOU HAVE THIS INFORMATION (Y/N)

Thermochemical data for C<sub>3</sub>H<sub>8</sub> was not included in the input data deck. We here assume that the user has in mind a reasonable figure for the LHV of typical hydrocarbon.

EQLBRM interrogates the user for the molecular composition of C<sub>3</sub>H<sub>8</sub>:

SPECIFY CHEMICAL COMPOSITION:

ENTER KG-ATOMS C PER KG-MOL C<sub>3</sub>H<sub>8</sub>

ENTER KG-ATOMS H PER KG-MOL C<sub>3</sub>H<sub>8</sub>

ENTER KG-ATOMS O PER KG-MOL C<sub>3</sub>H<sub>8</sub>

There is no oxygen in the C<sub>3</sub>H<sub>8</sub> molecule, so a null response is required.

ENTER KG-ATOMS N PER KG-MOL C<sub>3</sub>H<sub>8</sub>

YOU MAY SPECIFY EITHER:

- 1- STANDARD STATE ENTHALPY OF FORMATION
- 2- LOWER HEATING VALUE

WHICH VALUE? (1/2)

The user recalls that a typical LHV for hydrocarbon fuels is about 18,500 Btu/lbm, and decides to use this value.

SELECT UNITS:

- 1- KJ/KMOL
- 2- KJ/KG
- 3- BTU/LB
- 4- CAL/G

WHICH UNITS? (1-4)

ENTER LOWER HEATING VALUE

ENTER RELATIVE MOLES OF C<sub>3</sub>H<sub>8</sub>

Again, since this is the only fuel to be included, any nonzero value will do.

1.00

\*CURRENT FUELS DATA\*

FUEL	RELATIVE MOLES AMONG FUELS
C3H8	1.0000E+00

SELECT AN OPTION:

- 0- NO MORE CHANGES HERE
- 1- CHANGE RELATIVE MOLES OF AN EXISTING FUEL
- 2- ADD A NEW FUEL
- 3- REMOVE AN EXISTING FUEL
- 4- LIST ALL COMPOUNDS AVAILABLE IN THE THERMO LIBRARY

OPTION? (0-4)

No more changes are required, but the user decides to see what compounds are in the properties library:

4

\*COMPOUNDS AVAILABLE IN THERMO LIBRARY\*

CO	CO2	H	H2
H2O	N	NO	N2
O	OH	O2	NO2
CH4	C6H6	C6H6(L)	C7H8
C8H16	C8H18	C8H18(L)	C12H26
CH4O	C2H5OH	C3H8O	CH2
CH2O	C2H2	C2H4	C2H6
C3H8			

PRESS <RETURN> TO CONTINUE.

Note that C3H8 has been added to the list of recognised compounds. It will, however, be lost when EQLBRM is exited. The user must add thermochemical data for C3H8 to the input deck if C3H8 is to be used repeatedly. EQLBRM can accommodate up to 80 species, inclusive of those added interactively in the manner just demonstrated.

<return>

\*CURRENT FUELS DATA\*

FUEL	RELATIVE MOLES AMONG FUELS
C3H8	1.0000E+00

SELECT AN OPTION:

- 0- NO MORE CHANGES HERE
- 1- CHANGE RELATIVE MOLES OF AN EXISTING FUEL
- 2- ADD A NEW FUEL
- 3- REMOVE AN EXISTING FUEL
- 4- LIST ALL COMPOUNDS AVAILABLE IN THE THERMO LIBRARY

OPTION? (0-4)

No more changes are required.

☐ 0

\*\*\*CURRENT DATA STATUS\*\*\*

FUELS AND FUEL AMOUNTS :

FUEL	RELATIVE MOLES AMONG FUELS
C3H8	1.0000000
FUEL TEMP =	0.0000E-01 DEG- KELVIN
AIR TEMP =	0.0000E-01 DEG- KELVIN
PRESSURE =	0.0000E-01 ATMOSPHERES
A-F RATIO =	0.0000E-01 FUEL-AIR EQUIVALENCE RATIO

SELECT AN OPTION:

- 0- RUN WITH THIS DATA
- 1- CHANGE FUELS OR FUEL AMOUNTS
- 2- CHANGE FUEL TEMPERATURE
- 3- CHANGE AIR TEMPERATURE
- 4- CHANGE TEMPERATURE UNITS
- 5- CHANGE PRESSURE OR PRESSURE UNITS
- 6- CHANGE AIR-FUEL RATIO OR RATIO UNITS

OPTION NUMBER? (0-6)

The user wishes to work with Celsius as temperature units.

☐ 4

SELECT AN OPTION:

- 1- CHANGE UNITS TO KELVIN
- 2- CHANGE UNITS TO CELSIUS
- 3- CHANGE UNITS TO FAHRENHEIT
- 4- CHANGE UNITS TO RANKINE

OPTION? (1-4)

☐ 2

\*\*\*CURRENT DATA STATUS\*\*\*

FUELS AND FUEL AMOUNTS :

FUEL	RELATIVE MOLES AMONG FUELS
C3H8	1.0000000
FUEL TEMP =	0.0000E-01 DEG- CELSIUS
AIR TEMP =	0.0000E-01 DEG- CELSIUS
PRESSURE =	0.0000E-01 ATMOSPHERES
A-F RATIO =	0.0000E-01 FUEL-AIR EQUIVALENCE RATIO

SELECT AN OPTION:  
 0- RUN WITH THIS DATA  
 1- CHANGE FUELS OR FUEL AMOUNTS  
 2- CHANGE FUEL TEMPERATURE  
 3- CHANGE AIR TEMPERATURE  
 4- CHANGE TEMPERATURE UNITS  
 5- CHANGE PRESSURE OR PRESSURE UNITS  
 6- CHANGE AIR-FUEL RATIO OR RATIO UNITS

OPTION NUMBER? (0-6)

The user notes that fuel and air use the same units for temperature. Again, order is unimportant, but the user chooses to work top-down through the menu. Next in the menu is fuel temperature selection.

**2**

ENTER TEMPERATURE OF FUEL MIXTURE, DEG- CELSIUS

The user responds with the desired fuel temperature.

**125.00**

\*\*\*CURRENT DATA STATUS\*\*\*

FUELS AND FUEL AMOUNTS :  
 FUEL                      RELATIVE MOLES AMONG FUELS  
 C3H8                      1.0000000  
 FUEL TEMP = 1.2500E+02 DEG- CELSIUS  
 AIR TEMP = 0.0000E-01 DEG- CELSIUS  
 PRESSURE = 0.0000E-01 ATMOSPHERES  
 A-F RATIO = 0.0000E-01 FUEL-AIR EQUIVALENCE RATIO

SELECT AN OPTION:  
 0- RUN WITH THIS DATA  
 1- CHANGE FUELS OR FUEL AMOUNTS  
 2- CHANGE FUEL TEMPERATURE  
 3- CHANGE AIR TEMPERATURE  
 4- CHANGE TEMPERATURE UNITS  
 5- CHANGE PRESSURE OR PRESSURE UNITS  
 6- CHANGE AIR-FUEL RATIO OR RATIO UNITS

OPTION NUMBER? (0-6)

**3**

ENTER TEMPERATURE OF AIR, DEG- CELSIUS

Now the desired input air temperature is specified.

**375.00**

\*\*\*CURRENT DATA STATUS\*\*\*

FUELS AND FUEL AMOUNTS :  
 FUEL                      RELATIVE MOLES AMONG FUELS  
 C3H8                      1.0000000

FUEL TEMP = 1.2500E+02 DEG- CELSIUS  
AIR TEMP = 3.7500E+02 DEG- CELSIUS  
PRESSURE = 0.0000E-01 ATMOSPHERES  
A-F RATIO = 0.0000E-01 FUEL-AIR EQUIVALENCE RATIO

SELECT AN OPTION:

- 0- RUN WITH THIS DATA
- 1- CHANGE FUELS OR FUEL AMOUNTS
- 2- CHANGE FUEL TEMPERATURE
- 3- CHANGE AIR TEMPERATURE
- 4- CHANGE TEMPERATURE UNITS
- 5- CHANGE PRESSURE OR PRESSURE UNITS
- 6- CHANGE AIR-FUEL RATIO OR RATIO UNITS

OPTION NUMBER? (0-6)

Still working arbitrarily top-down, only options 5 and 6 remain to be exercised before the dataset is complete.

**5**

SELECT AN OPTION:

- 1- SAME UNITS, NEW PRESSURE
- 2- CHANGE UNITS TO KILO PASCALS
- 3- CHANGE UNITS TO P.S I.
- 4- CHANGE UNITS TO ATMOSPHERES
- 5- CHANGE UNITS TO BAR

OPTION? (1-5)

Note that entering either a "1" or a "4" would have the same effect here.

**1**

ENTER PRESSURE, IN ATMOSPHERES

**4.50**

\*\*\*CURRENT DATA STATUS\*\*\*

FUELS AND FUEL AMOUNTS :

FUEL	RELATIVE MOLES AMONG FUELS
C3H8	1.0000000

FUEL TEMP = 1.2500E+02 DEG- CELSIUS  
AIR TEMP = 3.7500E+02 DEG- CELSIUS  
PRESSURE = 4.5000E+00 ATMOSPHERES  
A-F RATIO = 0.0000E-01 FUEL-AIR EQUIVALENCE RATIO

SELECT AN OPTION:

- 0- RUN WITH THIS DATA
- 1- CHANGE FUELS OR FUEL AMOUNTS
- 2- CHANGE FUEL TEMPERATURE
- 3- CHANGE AIR TEMPERATURE
- 4- CHANGE TEMPERATURE UNITS
- 5- CHANGE PRESSURE OR PRESSURE UNITS
- 6- CHANGE AIR-FUEL RATIO OR RATIO UNITS



OPTION NUMBER? (0-6)

The only null data left is the air-fuel ratio.

SELECT AN OPTION:

- 1- SAME UNITS, NEW RATIO
- 2- CHANGE UNITS TO KG AIR/KG FUEL
- 3- CHANGE UNITS TO KG FUEL/KG AIR
- 4- CHANGE UNITS TO MOLS AIR/MOLS FUEL
- 5- CHANGE UNITS TO MOLS FUEL/MOLS AIR
- 6- CHANGE UNITS TO FUEL-AIR EQUIVALENCE RATIO

OPTION? (1-6)

Note that either a "1" or a "6" will have the same effect here.

ENTER FUEL-AIR EQUIVALENCE RATIO

\*\*\*CURRENT DATA STATUS\*\*\*

FUELS AND FUEL AMOUNTS :

FUEL	RELATIVE MOLES AMONG FUELS
C3H8	1.0000000
FUEL TEMP =	1.2500E+02 DEG- CELSIUS
AIR TEMP =	3.7500E+02 DEG- CELSIUS
PRESSURE =	4.5000E+00 ATMOSPHERES
A-F RATIO =	1.1000E+00 FUEL-AIR EQUIVALENCE RATIO

SELECT AN OPTION:

- 0- RUN WITH THIS DATA
- 1- CHANGE FUELS OR FUEL AMOUNTS
- 2- CHANGE FUEL TEMPERATURE
- 3- CHANGE AIR TEMPERATURE
- 4- CHANGE TEMPERATURE UNITS
- 5- CHANGE PRESSURE OR PRESSURE UNITS
- 6- CHANGE AIR-FUEL RATIO OR RATIO UNITS

OPTION NUMBER? (0-6)

The user has now specified all input conditions of the problem.

RUN WITH THIS DATA: ARE YOU SURE? (Y/N)

The user has double-checked all the items on the menu, so as to avoid wasting computer time on bad input data.

EQLBRM executes the dataset and presents the solution:

\*\*\*\*\*  
OUTPUT  
\*\*\*\*\*

\*\*\* ADIABATIC EQUILIBRIUM AT CONSTANT PRESSURE AND ENTHALPY \*\*\*

PRESSURE= 4.500E+00 ATMOSPHERES  
TEMPERATURE = 2007.09 DEGREES CELSIUS  
FUEL-AIR EQUIVALENCE RATIO = 1.100

SPECIES NAME ("I")	MOLE NUMBER (MOL-I/G-X)	MOLE FRACTION (MOL-I/MOL-X)	MASS FRACTION (G-I/G-X)	EMISSION INDEX (G-I/KG-FUEL)
CO	1.080E-03	2.993E-02	3.026E-02	3.026E+01
CO2	3.409E-03	9.444E-02	1.500E-01	1.500E+02
H	1.407E-05	3.899E-04	1.418E-05	1.418E-02
H2	3.274E-04	9.071E-03	6.600E-04	6.600E-01
H2O	5.632E-03	1.560E-01	1.015E-01	1.015E+02
N	4.476E-10	1.240E-08	6.269E-09	6.269E-06
NO	1.784E-05	4.944E-04	5.354E-04	5.354E-01
N2	2.556E-02	7.083E-01	7.161E-01	7.161E+02
O	1.125E-06	3.118E-05	1.800E-05	1.800E-02
OH	3.805E-05	1.054E-03	6.472E-04	6.472E-01
O2	8.201E-06	2.272E-04	2.624E-04	2.624E-01

DO YOU WANT A HARD COPY OF YOUR INPUT AND OUTPUT? (Y/N)

The user elects to make a hardcopy of both the input and output datasets.

☒ Y

DATA AND RESULTS ARE BEING APPENDED TO  
FILE "EQLOUT.LST" IN YOUR DIRECTORY.

The hard copy output is directed to logical unit 2. System-specific commands must be executed at run time (or added to the source code) to assign this unit to the file "EQLOUT.LST," or directly to an output device.

## 2.3 Debugging

If improper operation of EQLBRM is suspected, a debugging feature can be brought up by "un-commenting" the appropriate source code statements near the top of the main routine. With this feature restored, an interactive choice of debugging level (1-5) can be selected, which can be used (together with the source code listing) to discover implementation or source code transcription errors.

## 2.4 FORTRAN Language and Availability

Program EQLBRM was developed on a Digital Equipment Corporation PDP 11/23 computer. The source code is in 1966 ANSI-standard FORTRAN IV, and runs

without modification (except for system-specific I/O statements in the main routine KEYBRD) on VAX and IBM computers.

Source codes and the required data file EQLBRM.DAT are available from COSMIC, University of Georgia, Athens, Georgia 30602.

### 3. THERMOCHEMICAL DATA

The thermochemical data for elements and for nonelemental molecular species are taken directly from the NASA element and thermochemical data files (ref. 1).

In the EQLBRM.DAT data file, the ELEMENTS code word and elemental data must precede the THERMO code word and thermochemical data. The format for input data are summarized in tables I and II:

TABLE I. - ELEMENTS INPUT RECORDS

Order	Contents	Format	Record Columns
First	ELEMENTS	3A4	1 to 8
Any	One record each distinct element present in the chemical system. Each record contains:		
	1) Atomic symbol of element-- must agree with that used in THERMO data.	A2	1 to 2
	2) Atomic weight of the element	F10.6	10 to 19
	3) Valence or oxidation state of the element (positive, negative or zero).	F10.6	20 to 29
	See Note A		
Last	Blank record card	-----	all

Note A: EQLBRM is limited to ten distinct elements.

TABLE II. - THERMO INPUT RECORDS

Order	Contents	Format	Card Columns
First	THERMO	3A4	1 to 6
See Note B	Sets of four records in sequence for each species in the chemical system. The record formats for each set are, in order:		
First in set	1) Molecular symbol or name of species	3A4	1 to 12
	2) Date	2A3	19 to 24
	3) Atomic symbols and formula	4(A2,F3.0)	
	4) Phase (gas only, letter G)	A1	45
	5) Temperature	2F10.3	46 to 65
	6) Integer 1	I15	80
Second in set	1) Coefficients ( $z_i$ , $i = 1,5$ ) for upper temperature range. See Note A.	5E15.8	1 to 75
	2) Integer 2	I5	80
Third in set	1) Coefficients $z_6$ and $z_7$ for upper temperature range, and $z_1$ , $z_2$ and $z_3$ for lower. See Note A.	5E15.8	1 to 75
	2) Integer 3	I5	80
Fourth in set	1) Coefficients ( $z_i$ , $i = 4,7$ ) for low temperature interval. See Note A.	4E15.8	1 to 60
	2) Integer 4	I20	80
	See Note C	I20	80
Last	Blank record		

Note A: Coefficients ( $z_i$ ,  $i = 1,7$ ) correspond to the following equations for constant-pressure specific heat capacity, enthalpy, and entropy:

$$\frac{C_p}{R} = z_1 + z_2 T + z_3 T^2 + z_4 T^3 + z_5 T^4$$

$$\frac{h}{RT} = z_1 + \frac{z_2 T}{2} + \frac{z_3 T^2}{3} + \frac{z_4 T^3}{4} + \frac{z_5 T^4}{5} + \frac{z_6}{T}$$

$$\frac{s^\circ}{R} = z_1 \log T + z_2 T + \frac{z_3 T^2}{2} + \frac{z_4 T^3}{3} + \frac{z_5 T^4}{4} + z_7$$

ORIGINAL PAGE IS  
OF POOR QUALITY

The individual species enthalpy  $h$  include the standard-state enthalpy of formation and the sensible enthalpy. The individual species entropy  $s^\circ$  is for a pressure of one atmosphere.

Note B: The first two sets must be molecular nitrogen  $N_2$  and molecular oxygen  $O_2$ , the only constituents of air assumed in EQLBRM. All polyatomic fuel data-sets must reside at the end of the THERMO data file.

Note C: EQLBRM is limited to 80 distinct atomic and/or molecular species, including those entered interactively at run time.

#### 4. REFERENCES

1. Gordon, S. and McBride B., Computer Program for Calculation of Complex Chemical Equilibrium Compositions, NASA SP-273 (1971).
2. Pratt, D. T. "Calculation of Chemically Reacting Flows with Complex Chemistry," Studies in Convection, Vol. II, B. E. Launder, Ed., Academic Press (1976).
3. Smoot, L. D. and Pratt, D. T., Eds., Pulverized Coal Gasification and Combustion, Plenum Press (1979).
4. Pratt, D. T. and Wormeck, J. J., "CREK: A Computer Program for Calculation of Combustion Reaction Equilibrium and Kinetics in Laminar or Turbulent Flows," Washington State University Report WSU-ME-TEL-76-1 (1976).
5. Reynolds, W. C., STANJAN: Interactive Computer Programs for Chemical Equilibrium Analysis, Department of Mechanical Engineering, Stanford University, January (1981).